

Car-Parrinello and path integral molecular dynamics study of the hydrogen bond in the acetic acid dimer in the gas phase.

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Streszczenie

In the paper are described studies of the double proton transfer (DPT) processes in the cyclic dimer of acetic acid in the gas phase using Car-Parrinello (CPMD) and path integral molecular dynamics (PIMD). Structures, energies and proton trajectories have been determined. The results show the double proton transfer in 450 K. In the classical dynamics (CPMD) a clear process mechanism can be identified, where asynchronized DPT arises due to coupling between the O-H stretching oscillator and several low energy intermolecular vibrational modes. The DPT mechanism is also asynchronous when quantum tunneling has been allowed in the simulation. It has been found that the calculated values of barrier height for the proton transfer depends very strongly on the used approaches. Barrier received from the free-energy profile at the CPMD level is around 4.5 kcal mol⁽⁻¹⁾ whereas at the PIMD level is reduced to 1 kcal mol⁽⁻¹⁾. The nature of bonding in acetic acid dimer and rearrangement of electron density due to the proton movement has been also studied by the topological analysis of Electron Localization Function and Electron Localizability Indicator function

Adres publiczny

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